

Acute Oral Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (Non-regulatory)
Type	LD50
GLP	Pre-GLP
Year	1963
Species/Strain	Rat ■ Sprague-Dawley
Sex	Male
#/sex/dose	5
Vehicle	Corn oil (1.0 % or 10 % v/v)
Route of Admin	Oral Gavage
Doses	34.6, 120, 417, 1450, 5000, or 10,000 mg/kg
• Dose/time	Single dose following 3-4 hour-fast
• Post Dose Observation Period	1, 4, and 24 hours postdosing and daily for 14 Days
Results	
• LD50	>10 g/kg
• Remarks	One animal at the 1450 mg/kg dose level died on day 11. No toxic signs were observed prior to death and a normal body weight-gain was recorded at death. Postmortem examination showed congestion of the lungs, kidneys, adrenals, and pancreas, and gaseous distention of the stomach and large intestine at the time of death. All other animals showed no gross pathology following termination. Principal toxic effects seen only at the 10,000 mg/kg dose were depression, ataxia, sprawling of limbs and depressed righting reflex only at the 24-hour observation.
• Conclusion	The acute oral LD50 for C6 branched and linear alkyl acetate ester in male Sprague-Dawley rats is >10 g/kg.
Data Quality	1 ■ Reliable study without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Hazleton Laboratories Incorporated, Falls Church, VA, USA, Project # 38355.

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Acute Oral Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (EU Annex V, B.1 and OECD 401)
Type	Limit
GLP	Yes
Year	1995
Species/Strain	Rat • Crl:CDBR
Sex	Male & Female
#/sex/dose	5
Vehicle	None
Route of Admin	Oral Gavage
Doses	2000 mg/kg
• Doses/time	Single
• Post Dose Observation Period	14 Days
Results	
• LD50	>2 glkg
• Remarks	There was one female death on Day 0 at the 2-hour observation considered to be the result of test material aspiration during dosing. Clinical signs of toxicity were limited to nasal, oral and/or ocular discharge, abdominal and/or anogenital staining, and/or soft stool in four males at the Day 0 interval. One male and 4 females were free of abnormalities during the entire study. No gross abnormalities were seen at postmortem examination.
• Conclusion	C6 branched and linear alkyl acetate ester, did not elicit signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the male animals on Day 0. There was one female death on Day 0, but the death was the result of test material aspiration, not toxicity.
Data Quality	1 • Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, <u>Acute Oral Toxicity Test in the Rat</u> ; Project # 101501.

Acute Dermal Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Pre-GLP
Year	1963
Species/Strain	Rabbit (albino)
Sex	Male & Female
#/sex/dose	1
Vehicle	None
Route of Admin	Dermal Application
Doses	50, 200, 794 or 3160 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>3.16 glkg
• Remarks	Two animals, 200 and 3160 mg/kg dosage levels, showed soft feces or diarrhea for two to four days. One animal, 794 mg/kg dosage level, showed diarrhea during the second week and weight loss at termination. All other animals were normal and showed body weight gains. There were no gross pathological findings at the study termination.
• Conclusion	C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Hazleton Laboratories, Inc., Falls Church, VA, USA; Project # 38355.

Acute Dermal Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (EU Annex V, 8.3; OECD 402)
Type	Limit
GLP	Yes
Year	1995
Species/Strain	Rabbit - New Zealand White
Sex	Male & Female
#/sex/dose	5
Vehicle	None
Route of Admin	Dermal
Doses	2000 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>2 g/kg
• Remarks	There were no signs of systemic toxicity. Slight dermal irritation was noted in all animals, with the most severe response being observed at the Day 1 observation interval. At post mortem examination, all animals had desquamation at the dose site. In general, dermal responses were considered minimal and transient in nature.
• Conclusion	C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, <u>Acute Dermal Toxicity Study in the Rabbit</u> , Project # 101506.

Genetic Tox In Vitro

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	EU Annex V, 8.14; OECD 471
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	Yes
Year	1995
Species/Strain	S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	
• Species/cell type	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	250, 500, 1000, 2000, and 3000 µg/plate
Vehicle	DMSO
Remarks for Test Conditions	<p>There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 250, 500, 1000, 2000, and 3000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.</p>

Results

- **Remarks**

C6 branched and linear alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

Toxicity was observed in both the initial and repeat assays in the following strains and dose levels: TA96 at 2000 $\mu\text{g/plate}$ without metabolic activation, and at 3000 $\mu\text{g/plate}$ with and without metabolic activation; TA100 at 2000 and 3000 $\mu\text{g/plate}$ with and without metabolic activation; TA1535 at 2000 $\mu\text{g/plate}$ without metabolic activation; TA1 537 at 250, 500, 1000, 2000, and 3000 $\mu\text{g/plate}$ without metabolic activation; and TA1 538 at 1000 and 2000 $\mu\text{g/plate}$ without metabolic activation, and at 3000 $\mu\text{g/plate}$ with and without metabolic activation. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.
- **Conclusion**

C6 branched and linear alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, but was toxic in all strains tested under the conditions of this study.
- Data Quality**

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
- Reference**

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Assay; Project # 101525.

Genetic Tox In Vitro

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Galloway, et al, <u>Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories.</u> Environ. Mutagen. 7:1-51, 1985.
Type	In Vitro Chromosomal Aberration Assay in CHO Cells
System of Testing	Cultured Chinese hamster ovary (CHO) cells
GLP	Yes
Year	1995
Remarks for Test Conditions	Treatment group doses (14 total in initial and repeat assays) ranged from 250-480 µg/mL in the 20-hour initial test; 230-550 µg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 350-480 µg/mL in the 20-hour initial assay and ranging from 380-550 µg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate). Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.
Results	C6 branched and linear alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was no evidence of a positive dose response nor of any treated group being different from the control in these analyses. For the repeat harvest, the high dose group (550 µg/mL) was statistically different from the vehicle control (p<0.05). However, this statistically significant finding (6.5% aberrant cells) was not reproducible. No increase was observed at the 44-hour harvest time. In addition, no increase was observed in the initial assay with metabolic activation at similar dose levels. There was no statistically significant finding in the 44-hour harvest.
Remarks	C6 branched and linear alkyl acetate ester, reduced cell survival by at least 50% when compared to the vehicle control in the repeat assay: 20- hour harvest without activation and 44-hour harvest with and without metabolic activation. All negative and positive controls used in this study performed in an appropriate manner.

Conclusion	C6 branched and linear alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 550 $\mu\text{g/mL}$ with and 430 $\mu\text{g/mL}$ without metabolic activation.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, <u>In Vitro Chromosomal Aberration Assay in CHO Cells</u> , Project # 101532.

Repeated Dose Oral Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	EU Annex V, 8.7; OECD 407
Type	28-Day Repeated Dose Oral Toxicity
GLP	Yes
Year	1995
Species/Strain	Rat - CrI:CD BR
Sex	Male & Female
#/sex/dose	5
Vehicle	Corn Oil
Route of Admin	Gavage
Duration of Test	28-Day
Doses	0, 100, 500, and 1000 mg/kg/day
• Volume	5 ml/kg
Results	
• NOAEL	1000 mg/kg/day
• Conclusion	Oral administration of C6 branched and linear alkyl acetate ester daily to rats for 28 days did not produce any signs of overt systemic toxicity at any dose level tested. There were no treatment-related clinical in-life, gross postmortem or microscopic findings (including adrenal glands, heart, kidneys, liver, lung, spleen, testes and ovaries); no treatment-related mortality; and no adverse effects on body weight, food consumption, clinical laboratory parameters, or organ weights.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, <u>28-Day Repeated Dose Oral Toxicity Study in the Rat</u> , Project # 101570.

Acute Dermal Toxicity

Test Substance	C6-C8 branched alkyl acetate ester
CAS #	90438-79-2
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>3.16 g/kg
• Remarks	There were no overt signs of systemic toxicity. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. Erythema was noted in all animals at 24 hours, ranging from moderate to severe, and regressed in all animals throughout the study. On Day 14, five of six animals showed very slight erythema and one had no signs of erythema. Edema was evident in all but one animal at 24 hours and by Day 14 all but one animal was free of signs of edema. Desquamation was evident in five animals on Day 14. All animals survived to termination of the study and increased in body weight. There were no significant findings at the postmortem gross examination.
• Conclusion	C6-C8 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

ExxonMobil Chemical Company
Alkyl Acetate C6 - C13 Category

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C6-C8 Branched Alkyl Acetate Ester.
Project # 321106.

Genetic Tox *In Vitro*

Test Substance	C6-C8 branched alkyl acetate ester
CAS #	90438-79-2
Method	EU Annex V, B.14; OECD 471
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	Yes
Year	1997
Species/Strain	S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	
• Species/cell type	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	<u>50</u> , 100, 200, 400, 600, and <u>800</u> $\mu\text{g/plate}$ (<u> </u> repeat assay only; <u> </u> initial assay only)
Vehicle	DMSO
Remarks for Test Conditions	<p>There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 100, 200, 400, 600, and 800 $\mu\text{g/plate}$ of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 $\mu\text{g/plate}$ for all strains with S9; 2-nitrofluorine (2-NF) at 5 $\mu\text{g/plate}$ for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 $\mu\text{g/plate}$ for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 $\mu\text{g/plate}$ for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 μl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37\pm 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.</p>
Results	
• Remarks	C6-C8 branched alkyl acetate ester, did not induce significant increases in revertant colonies (\geq 3 times the vehicle controls) in any of the tested

strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a **3-fold** increase in revertant colonies in their respective strains.

Toxicity was observed in the initial assay in the following dose levels and strains: at 100 $\mu\text{g/plate}$ TA1 537 (+S9), $\geq 200 \mu\text{g/plate}$ in TA1 00 (-S9), TA1 535 (+S9), TA1 537 (-S9), TA1 538 (\pm S9); $\geq 400 \mu\text{g/plate}$ in TA98 (\pm S9), TA1 535 (-S9), TA1 537 (+S9), and $\geq 600 \mu\text{g/plate}$ in TA100 (+S9). In the repeat assay, toxicity was observed at doses $> 400 \mu\text{g/plate}$ in TA1 00 (-S9) and TA1 537 (-S9), and at 600 $\mu\text{g/plate}$ in TA98 (-S9), TA1 535 (-S9), TA1 537 (+S9), and TA1 538 (\pm S9). The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

• **Conclusion**

C6-C8 branched **alkyl** acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested, even at doses that produced evidence of toxicity.

Data Quality

1 ■ Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Assay with C6-C8 Branched Alkyl Acetate Ester. Project # 164025.

Genetic Tox *In Vitro*

Test Substance	C6-C8 branched alkyl acetate ester
CAS #	90438-79-2
Method	Galloway, et al, <u>Development of a standard <i>protocol</i> for <i>in vitro</i> cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories.</u> Environ, Mutagen. 7:1-51, 1985.
Type	In Vitro Chromosomal Aberration Assay in CHO Cells
System of Testing	Cultured Chinese hamster ovary (CHO) cells
GLP	Yes
Year	1997
Remarks for Test Conditions	Treatment group doses (11 total in initial and repeat assays) ranged from 80-240 µg/mL in the 20-hour initial test; 40-200 µg/mL in the 20- and 44- hour repeat assays. S9 activation was used in doses ranging from 80-240 µg/mL in the 20-hour initial assay and ranging from 40-200 µg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate). Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.
Results	C6-C8 branched alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was a notable decrease in the percent cell confluency at concentrations ≥ 180 µg/mL with activation and at concentrations ≥ 140 µg/mL without activation. Cell morphology and mitotic indices were acceptable at or below these levels and cell death was prevalent above these levels. For the repeat assay, there were no statistically significant dose-related trends in the percentage of aberrant cells and none of the test concentrations were statistically different than the vehicle control in the 20 or 44 hour activated or nonactivated series. The percentage of aberrant cells in the vehicle control groups ranged from 1% to 2.0% , and the percentage of aberrant cells in the treated groups ranged from 0.0% to 2.6% for the 20 and 44 hour activated and nonactivated series.
Remarks	All negative and positive controls used in this study performed in an appropriate manner.
Conclusion	C6-C8 branched alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 180 µg/mL with and 140 µg/mL without metabolic activation.

Data Quality 1 • Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference Exxon Biomedical Sciences, inc., East Millstone, NJ, USA, In Vitro Chromosomal Aberration Assay in CHO Cells with C6-C8 Branched Alkyl Acetate Ester. Project # 164032.

Acute Dermal Toxicity

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>3.16 glkg
• Remarks	Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. One animal was sacrificed on Day 11 due to severe weight loss. The surviving five animals showed slight weight gain through the study. Dermal evaluations ranged from no erythema to moderate to severe. Edema scores ranged from no edema to slight edema. Desquamation was noted in four animals during the study. The animal terminated on Day 11 revealed kidney discoloration, small spleen, cecum and ileum, and brown material in the stomach. The remaining five animals showed no abnormalities at necropsy.
• Conclusion	C7-C9 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 • Reliable without Restrictions, No circumstances occurred that would have affected the quality or integrity of the data.

ExxonMobil Chemical Company
Alkyl Acetate C6 - Cl 3 Category

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study
in the Rabbit with C7-C9 Branched Alkyl Acetate Ester.
Project # 330306.

Genetic Tox In Vitro

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	FIFRA 84-2
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	Yes
Year	1994
Species/Strain	S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	
• Species/cell type	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	25, 50, 100, 200, 400, and 600 µg/plate (___ repeat assay only; ___ initial assay only)
Vehicle	DMSO
Remarks for Test Conditions	<p>There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 25, 50, 100, 200, 400, or 600 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.</p>

Results

• Remarks

C7-C9 branched alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was observed for all five tester strains with an without metabolic activation in both the initial and repeat assays, except for tester strain **TA1535** with metabolic activation for the repeat assay. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

• Conclusion

C7-C9 branched alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested.

Data Quality

1 ■ Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay with **C7-C9** Branched Alkyl Acetate Ester. Project # 168825.

Genetic Tox *In Vivo*

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	TSCA 798.5395
Type	In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method
GLP	Yes
Year	1994
Species	Mouse
Strain	Crl:CD-1 (VAF/Plus)
Sex	Males and Females
Number	5/sex/dose
Route of Administration	Oral Gavage
Doses/time	0.825, 1.25, and 2.5 grams/kg / Single dose
Test Period	24, 48 and 72 hours
Vehicle	Corn Oil
Positive Control	Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage
Remarks	<p>The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei (1000 polychromatic erythrocytes/animal were evaluated).</p>
Results	<p>A statistically significant increase in the mean number of micronucleated polychromatic erythrocytes was not seen at any dose level. Cytotoxicity, shown by a dose-related decrease in the percentage of polychromatic erythrocytes, was observed for both sexes at the 48-hour sampling time (regression coefficient $p < 0.01$). The two highest dose groups were statistically different from the vehicle control. Both the positive</p>

(cyclophosphamide) and negative (vehicle carrier) controls responded in an appropriate manner.

Remarks

The test material is considered to be toxic to bone marrow in CD-1 mice under the conditions of this test based on the decrease in the mean percent of polychromatic erythrocytes at the **48-hour** sampling time.

Conclusion

C7-C9 branched **alkyl** acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method with **C7-C9** Branched Alkyl Acetate Ester. Project # 168830.

Repeated Dose Oral Toxicity

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	EPA TSCA 798.2650
Type	13-Week Repeated Dose Oral Toxicity
GLP	Yes
Year	1985
Species/Strain	Rat - Sprague-Dawley
Sex	Male & Female
#/sex/dose	20
Vehicle	None
Route of Admin	Gavage
Duration of Test	90-Day
Doses	0, 0.1, 0.5, and 1.0 g/kg/day
• Volume	≤ 1.11 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1.11 ml/kg)
• Remarks	Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.
Results	
• NOAEL	1.0 g/kg/day
• Remarks	Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.
• Conclusion	Oral administration of C7-C9 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical

observations were primarily oral and dermal irritation (no clear **dose-response**). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels for the interim and terminal evaluations. At the terminal sacrifice, there were no biologically significant differences between treated and control animals for the measured clinical chemistries. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. All other organ weights were comparable to control values. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix, and corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, **NJ**, USA, Subchronic Oral Gavage Study in Rats; Project # 230370.

Developmental Toxicity / Teratogenicity

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	EPA 798.4900 Guideline
Type	Developmental Toxicity
GLP	Yes
Year	1985
Species	Rat
Strain	Sprague-Dawley
Route of Admin	Oral Gavage
Doses/Concentration	0, 100, 500 and 1000 mg/kg
Sex	Female
Exposure Period	Gravid Day 6-15
Frequency of Treatment	Single Dose Daily
Control Group	Sham-Treated with distilled water at 1000 mg/kg
Duration of Test	Gravid Day 20
Statistical Methods	Maternal body weight, body weight change, food consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.
#/sex/dose	22 Mated Females
Vehicle	None

Results

- **Maternal NOEL** 100 mg/kg/day
- **Maternal NOAEL** 500 mg/kg/day
- **Pup NOEL** 500 mg/kg/day
- **Pup NOAEL** 500 mg/kg/day
- **Remarks** For the 1000 **mg/kg** group, there was a slightly increased incidence of malformations, although the different types of malformations, observed did not suggest a characteristic pattern of anomalies. No developmental toxicity was observed at the maternally toxic dose of 500 **mg/kg** or the maternally nontoxic dose of 100 **mg/kg**.
- **Conclusion** C7-C9 branched **alkyl** acetate ester, was administered at 0, 100, 500, and 1000 **mg/kg** on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen at the 500 and 1000 **mg/kg** doses as evidenced by decreases in body weight and food consumption. There was a slight increase in fetal malformations and embryotoxicity in the 1000 **mg/kg** group only; no adverse fetal effects were observed in the 100 and 500 **mg/kg** groups.
- Data Quality** 1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.
- Reference** Bio/Dynamics Inc., East Millstone, **NJ**, USA, Oral Teratology Study in Rats Project # 330334.

Acute Dermal Toxicity

Test Substance	C8-C10 branched alkyl acetate ester
CAS #	108419-33-6
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>3.16 g/kg
• Remarks	<p>Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. Erythema was noted in all animals at 24 hours and continued in four animals through Day 14. Edema was seen in three animals at 24 hours. No animals showed edema by the Day 7 evaluation. Desquamation was seen in one animal on Day 7, three animals on Day 10 and remained in two animals at the Day 14 termination. One male and two females at Day 7 and one male and one female showed slight decreases in body weight. Food consumption was reduced on Day 1 only. Postmortem examination revealed gallbladder and salivary gland abnormalities, kidney discoloration, a urinary bladder abnormality, hair in two stomachs and ano-genital staining.</p>
• Conclusion	C8-C10 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3.16 g/kg.

Data Quality

1 . Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Bio/dynamics inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C8-C10 Branched Alkyl Acetate Ester. Project # 330406.

Acute Dermal Toxicity

Test Substance	C9-C11 branched alkyl acetate ester
CAS #	108419-34-7
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1984
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>3.16 g/kg
• Remarks	Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. There were no deaths during the course of this study. Three of six animals gained weight during the study. Clinical in-life observations included ano-genital staining, ocular discharge, unthrifty coat, nasal discharge and poor food consumption. Erythema and edema were slight to well defined. Desquamation was also observed. Postmortem examination revealed kidney discoloration, an encapsulated salivary gland, an enlarged cervical lymph node and hair present in the stomach.
• Conclusion	C9-C11 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3.16 g/kg.
Data Quality	1 • Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C9-C11 Branched Alkyl Acetate Ester.
Project # 330506.

Acute Oral Toxicity

Test Substance	CI I-CI4 branched alkyl acetate ester
CAS #	108419-35-8
Method	Experimental
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rat (Sprague-Dawley)
Sex	Male & Female
#/sex/dose	5
Vehicle	None
Route of Admin	Oral Gavage
Doses	
• Doses/time	Single (18 Hr Fasted)
• Vol. Admin.	5.721 ml/kg (1 .1 - 1.9 ml)
• Post Dose Observation Period	14 Days
Results	
• LD50	>5 g/kg
• Remarks	There were no deaths during this study. Nine of 10 animals showed staining in the ano-genital area on Days 1 and 2, and for 1 animal on Day 3. Soft stool was noted for 1 animal at 6 Hrs PD and white gelatinous material on the penis was noted for 1 animal on Day 1. There were no observable abnormalities noted after the Day 3 observations. All animals except one showed an increase over pre-dose weights except one animal that appeared to have had an incorrect pre-dose weight recorded. Six of 10 animals showed no observable abnormalities during postmortem examination. Four animals showed lung discoloration typical of findings resulting from carbon dioxide asphyxiation.
• Conclusion	CI 1 -CI4 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the first 3 days.

Data Quality

1 ■ Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Bio/dynamics, East Millstone, NJ, USA, Acute Oral Toxicity Study in the Rat; Project # 330601.

Acute Dermal Toxicity

Test Substance	Cl 1 -C14 branched alkyl acetate ester
CAS #	108419-35-8
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1984
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• Doses/time	Single application / 24-Hour Occlusive Patch
• Post Dose Observation Period	14 Days
Results	
• LD50	>3.16 g/kg
• Remarks	There were no overt signs of systemic toxicity. Five of 6 rabbits showed slight body weight decreases at Day 7; only 2 animals continued to have decreased body weight at 14 days. Slight dermal irritation persisted in 4 of 6 test animals through termination of the study. In general, dermal responses were considered minimal and transient in nature. At post mortem examination, 3 of 6 animals showed no observable abnormalities. Liver and salivary gland discoloration was observed in one animal; kidney discoloration and spleen enlargement in another; and alopecia in the third animal.
• Conclusion	Cl I-C14 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Bio/dynamics Inc., East Millstone, NJ, USA, <u>Acute Dermal Toxicity Study in the Rabbit</u> ; Project # 330606.

Genetic Tox *In Vitro*

Test Substance	Cl I-Cl4 branched alkyl acetate ester
CAS #	108419-35-8
Method	FIFRA 84-2
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	Yes
Year	1994
Species/Strain	S. typhimurium / TA98, TA1 00, TA1 535, TA1 537, TA1 538
Metabolic Activation	
• Species/cell type	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	156, 312.5, 625, 1250, 2500, <u>5000</u> , and <u>10000</u> µg/plate (___ repeat assay only; == initial assay only)
Vehicle	DMSO
Remarks for Test Conditions	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA1 00, TA1 535, TA1537, and TA1 538. Each of the five strains was dosed with 156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1 538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA1 00, TA1 535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Results

• Remarks

CI I-CI4 branched alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was not observed. Test substance beading was observed for all tester strains, both with and without metabolic activation at 1250 through 10000 $\mu\text{g}/\text{plate}$. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

• Conclusion

CI I-CI4 branched alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested and was not toxic in any strain tested under the conditions of this study.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay; Project # 168925.

Genetic Tox *In Vivo*

Test Substance	Cl I -C14 branched alkyl acetate ester
CAS #	108419-35-8
Method	TSCA 798.5395
Type	In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method
GLP	Yes
Year	1994
Species	Mouse
Strain	CrI:CD-1 (VAF/Plus)
Sex	Males and Females
Number	5/sex/dose
Route of Administration	Oral Gavage
Doses/time	0.45, 0.90, and 1.80 grams/kg / Single dose
Test Period	24, 48 and 72 hours
Vehicle	Corn Oil
Positive Control	Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage
Remarks	<p>The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei (1 000 polychromatic erythrocytes/animal were evaluated).</p>
Results	<p>A dose-related decrease in the percentage of polychromatic erythrocytes was observed for the female 48-hour sampling time (regression coefficient $p<0.01$). However, none of the dose groups were statistically different from the control. The positive control (40 mg/kg cyclophosphamide) induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes ($p<0.01$)</p>

which indicates that the positive control is clastogenic and is responding in an appropriate manner. Vehicle carrier control values for the mean percent of polychromatic erythrocytes and for the mean percent of micronucleated polychromatic erythrocytes responded in an appropriate manner.

Remarks

The test material is considered to be toxic to bone marrow in CD-1 mice based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

Conclusion

Cl I-Cl4 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method, Project # 168930

Repeated Dose Oral Toxicity

Test Substance	Cl 1 -C14 branched alkyl acetate ester
CAS #	108419-35-8
Method	EPA TSCA 798.2650
Type	13-Week Repeated Dose Oral Toxicity
GLP	Yes
Year	1985
Species/Strain	Rat - Sprague-Dawley
Sex	Male & Female
#/sex/dose	20
Vehicle	None
Route of Admin	Gavage
Duration of Test	90-Day
Doses	0, 0.1, 0.5, and 1.0 g/kg/day
• Volume	≤ 1,111 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1.111 ml/kg)
• Remarks	Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.
Results	
• NOAEL	1.0 g/kg/day
• Remarks	Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.
• Conclusion	Oral administration of Cl 1 -Cl 4 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical

observations were primarily oral and dermal irritation (no clear **dose-response**). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels. At the terminal sacrifice, glucose values for the 0.5, and 1 .0 g/kg/day males were lower than controls and the total protein values for the 1 .0 g/kg/day females were higher than controls. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy in the mid- and high-dose male rats that were consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix/corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Subchronic Oral Gavage Study in Rats; Project # 252170.

Developmental Toxicity / Teratogenicity

Test Substance	Cl I-Cl4 branched alkyl acetate ester
CAS #	108419-35-8
Method	EPA 798.4900 Guideline
Type	Developmental
GLP	Yes
Year	1985
Species	Rat
Strain	Sprague-Dawley
Route of Admin	Oral Gavage
Doses/Concentration	0, 500, 1300, and 2500 mg/kg
Sex	Female
Exposure Period	Gravid Day 6-15
Frequency of Treatment	Single Dose Daily
Control Group	Sham-Treated with distilled water at 2.5 g/kg
Duration of Test	Gravid Day 20
Statistical Methods	Maternal body weight, body weight change, food consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.
#/sex/dose	22 Mated Females
Vehicle	None

Results

- **Maternal NOEL** 500 mg/kg/day
- **Maternal NOAEL** 500 mg/kg/day
- **Pup NOEL** 2500 mg/kg/day
- **Pup NOAEL** 2500 mg/kg/day

Remarks There were no statistically significant deleterious effects on survival, fetal body weight, crown-rump length or malformations at any dose.

Conclusion Cl I-Cl4 branched **alkyl** acetate ester was administered at 0, 500, 1300, and 2500 **mg/kg** on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen at the 1300 and 2500 **mg/kg** doses as evidenced by decreases in body weight. There were no statistically significant deleterious effects on fetal survival, body weight, or **crown-rump** length and no evidence of treatment-related malformations.

Data Quality 1 ■ Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference Bio/dynamics Inc., East Millstone, **NJ**, USA, Oral Teratology Study in Rats; Project # 352134.

Fish Acute Toxicity

Test Substance: CAS No. 88230-35-7, C6 branched and linear alkyl acetate ester

Method/Guideline: OECD 203

Year (guideline): 1992

Type (test type): Semi-Static Fish Acute Toxicity Test

GLP: Yes

Year (study performed): 1995

Species: Rainbow Trout (*Oncorhynchus mykiss*)

Analytical Monitoring: Yes (TOC)

Exposure Period: 96 hour

Statistical Method: Trimmed Spearman Karber Method

Test Conditions:

- Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.

Individual test concentrations were prepared by adding the test substance to 17L of laboratory blend water in 20L glass carboys. The solutions were mixed for 24 hours at test temp (13-17 Deg C) with a vortex of <1 0%. Mixing was performed using a magnetic stir plate and teflon stir bar (132 rpm). After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via a glass tube from the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.5L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Three replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF. Nominal treatment levels were control, 0.5, 1.3, 3.2, 8.0, and 20.0mg/L

Test temperature was 15.2 Deg C. Lighting was 62 to 69 ft. candles with gradual 16 hrs light and 8 hrs dark. Dissolved oxygen was 9.0 to 9.4mg/L for "new" solutions and 6.3 to 8.5mg/L for "old" solutions. The pH ranged from 7.4 to 7.7 for "new" solutions and 7.0 to 7.4 for "old" solutions.

Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.333g; mean total length=3.6cm; test loading=0.37g of fish/L.

Results:

96 hour **LL50** = 11 .9mg/L (95% **CI** 10.6 to 13.4) based upon nominal values.

Units/Value:

Results con't

Analytical method used was Total Organic carbon (TOC). The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Measured</u> <u>Conc. (mg/L)</u>	<u>Fish Total</u> <u>Mortality (@96 hrs)</u>
Control	0
0.5	0
1.3	0
3.2	0
8.0	1
20.0	15

*1 5 fish added at test initiation

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences Inc. 1995. Acute Fish Toxicity Test with Rainbow Trout. Study **#101558**.

Other (source):

ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance: CAS No. 88230-35-7; C6 branched and linear alkyl acetate ester

Method/Guideline: OECD 202

Year (guideline) 1992

Type (test type): Static Acute Daphnid Toxicity Test

GLP: Yes

Year (study performed): 1995

Species: Water Flea (Daphnia magna)

Analytical Monitoring: Yes (TOC)

Exposure Period: 48 hour

Statistical Method: Finney, D.J. **probit** procedure of SAS

Test Conditions:

- **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Individual treatment solutions were prepared as water accommodated fractions (**WAFs**). A WAF was prepared by adding test substance to **1.8L** of solution in a 2.0 liter aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was **<10%**. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle.

Test vessels were 125ml glass beakers filled with 140ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 5 organisms.

Nominal treatment levels were: control, **0.1, 0.5, 1 .0, 5.0**, and 1 0.0mg/L

Test temperature was 20.7 Deg C. Lighting was 58 to 59 ft candles with 16 hrs light and 8 hrs dark. Dissolved oxygen was 7.3 to **8.8mg/L**. The pH ranged from 7.3 to 8.3.

Organisms were supplied by in-house cultures; age = **<24** hours old. Parents age = 14 to 18 days old.

Results:

48 hour LL50 = 7.6mg/L (95% CI 5.9 to 10.7mg/L) based upon nominal values.

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was Total Organic Carbon (TOC).

<u>Nominal</u> <u>Conc. (mg/L)</u>	<u>Daphnia Total</u> <u>Mortality (@48 hrs)</u>
Control	1
0.1	2
0.5	1
1.0	3
5.0	5
10.0	14

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences, Inc. 1995. Acute Daphnid Toxicity Test. Study #1 01542B.

Other (source):

ExxonMobil Chemicals

Algal Toxicity

Test Substance:	CAS No. 88230-35-7, C6 branched and linear alkyl acetate ester
Method/Guideline:	OECD 201, Annex V
Year (guideline):	1992
Type (test type):	Algal Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species/Strain:	Fresh-Water Green Algae (<i>Selenastrum capricornutum</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Proc regression procedure of SAS, Anova procedure of SAS for NOEC
Test Conditions:	<p>Individual test treatment solutions were prepared as Water Accommodated Fractions (WAFs). Test material was added to 1.8L of algal media in 2.0L aspirator bottles. The mixing vessels were sealed with foil covered stoppers and mixed on magnetic stir plates with teflon coated stir bars for 24 hours at room temperature. After mixing the solutions were allowed to settle for one hour and the WAF was removed from the bottom of the mixing vessel via the port and used for testing. Test vessels were 125ml glass Erlenmeyer flasks that were completely filled (140ml) with treatment solution and inoculated with algae. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1.0×10^4 cells/ml. All test replicates were placed on a shaker table at 100 oscillations per minute during the study. To facilitate mixing, with no headspace, 10 glass beads were placed in each vessel. Biomass was calculated as the area under the growth curve. Nominal treatment levels were 8.0, 31.0, 62, 125, and 250mg/L</p> <p>Test temperature was 23.6 Deg. C. Lighting was continuous at 4300 to 4663 Lux. The pH was 7.5 at test initiation and ranged from 8.3 to 10.4 at test termination.</p>
Results:	
Units/Value:	96 hour EL50b=40.1 mg/L (biomass) 96 hour EL50gr=32.1 mg/L (growth rate)
Measurement (cells/growth)	72 & 96 hour NOELRb=31.0mg/L (biomass) 72 & 96 hour NOELRgr=8.0mg/L (growth rate)
	Analytical method used was Dissolved Organic Carbon (DOC). No excursions from the protocol were noted.

Results **con't**

Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.

Nominal
Conc. mg/L

Growth - 72 & 96 hr
(% Inhibition)

Mean Cell
Conc. - 96 hr
(cells/ml)

Control	n/a	n/a
8.0	1.2	-4.2*
31.0	8.4	-3.5*
62.0	80.2	84.4
125.0	94.5	97.2
250.0	99.9	100

8.8×10^5
1.1×10^6
1.1×10^6
2.6×10^4
9.6×10^3
3.4×10^3

n/a • Not applicable
● Stimulatory response

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences Inc. 1995. Algal Inhibition Test. Study #101567.

Other (source):

ExxonMobil Chemicals

Biodegradation

Test Substance: CAS No. 88230-35-7; C6 branched and linear alkyl acetate ester

Method/Guideline: USEPA TSCA 40 CFR 796.3100

Year (guideline) 1988

Type (test type): Aerobic Aquatic Biodegradation (Gledhill Shake Flask Test)

GLP: Yes

Year (study performed): 1994

Inoculum: Domestic activated sludge, raw sewage and soil

Exposure Period: 28 days

Test Conditions:

• **Note: Concentration prep., vessel type, replication, test conditions.**

Non acclimated activated sludge, sewage, soil, and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 2L Gledhill flasks located in the dark in an environmental chamber. Each test vessel was monitored for carbon dioxide via charcoal tube and air purging. Sampling was performed on Days 2, 3, 5, 7, 13, 19, and 28. Test material and positive control were tested in triplicate. Test material concentration was 30mg carbon/L. Aniline (positive control) concentration was 20 mg carbon/L. Test temperature was 19 to 23 Deg C.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Test material was readily biodegradable. Half-life was ≤ 2 weeks. By day 28, 76.9% degradation of the test material was observed. 10% biodegradation was achieved on approximately day 2, 50% biodegradation on approximately day 13. By day 7, $>60\%$ biodegradation of positive control was observed. No excursions from the protocol were noted. Biodegradation was based on theoretical Carbon Dioxide values and the cumulative Carbon Dioxide produced by the test substances.

<u>Sample</u>	% Degradation* <u>28y</u>	Mean % Degradation <u>(day 28)</u>
Test Substance	74.6, 82.0, 74.1	76.9
Aniline	86.5, 83.7, 83.9	84.7

* replicate data

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1994. Aerobic Aquatic Biodegradation, Gledhill Shake Flask Test. Study **#168687**.

Other (source): ExxonMobil Chemicals

Stability in Water

Test Substance:	CAS No. 88230-35-7; C6 branched and linear alkyl acetate ester
Method/Guideline:	OECD Guideline 111 and EC Annex V Guideline C.7
Year (guideline):	1992
Type (test type):	Hydrolysis (abiotic)
GLP:	Yes
Year (study performed):	1995
Exposure Period:	27- 45 days (definitive test)
Test Conditions:	<p>The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test of 95ug/ml at pH values of 4, 7, and 9 showed stability at pH 4 and 7. A definitive test was performed at 98 ug/ml and a pH value of 9 at varying temperatures (15 and 25 Deg C).</p> <p>A sufficient volume of test substance stock solution was added to a buffer solution to yield a nominal concentration of 98 ug/ml (less than half of expected maximum water solubility concentration). Test samples were stored in the dark in laboratory incubators and the temperature recorded daily.</p> <p>Test vessels were sterilized VOA vials containing a buffer solution with the test substance and no headspace.</p> <p>Test substance concentrations were measured by GC-FID.</p>
Results:	Half life at pH 9 and 25 Deg C = 13 days.
Units/Value:	Half life at pH 9 and 15 Deg C = 36 days.
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method.	<p>Test substance was stable at pH 4 and pH 7. Less than 5% degradation was measured over a period of 5 days at these two pH values.</p> <p>Hydrolysis of test substance occured at pH 9, with 35% degradation observed after day 1 and 95% after day 5.</p>
Conclusion:	Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 25 Deg C and the pH is at or below 7.
Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1995 Abiotic Degradation Hydrolysis as a Function of pH . Study #101 590.
Other (source):	ExxonMobil Chemicals

Fish Acute Toxicity

Test Substance: CAS No. 90438-79-2, C6 - C8 branched alkyl acetate ester

Method/Guideline: OECD 203

Year (guideline): 1992

Type (test type): Semi-Static Fish Acute Toxicity Test

GLP: Yes

Year (study performed): 1997

Species: Rainbow Trout (*Oncorhynchus mykiss*)

Analytical Monitoring: Yes

Exposure Period: 96 hour

Statistical Method: Trimmed Spearman Karber Method

Test Conditions:

- Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.

Individual test concentrations were prepared by adding the test substance, weighed on teflon disks, to 12 L of laboratory blend water in 13L glass aspirator bottles. The solutions were mixed for 24 hours at room temp (20-24 Deg C) with a vortex of <10% (3 cm vortex). Mixing was performed using a magnetic stir plate and teflon stir bar. After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via port at the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.0L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Two replicates of each concentration were tested, each containing 5 fish.

Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Nominal treatment levels were control, 2.0, 4.5, 10.0, 23.0, and 50.0mg/L, which measured: 1.2, 1.49, 5.39, 21 .1, and 43.6mg/L, respectively, and are based on the mean of samples taken from the new and old solutions.

Test temperature was 13.6 Deg C. Lighting was 16 hrs light and 8 hrs dark. Dissolved oxygen was 8.3 to 10.4mg/L for "new" solutions and 4.5 to 7.9mg/L for "old" solutions. The pH ranged from 7.3 to 8.4 for "new" solutions and 6.7 to 7.6 for "old" solutions. Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.319g; mean total length=3.5cm; test loading=0.399g of fish/L.

Results:

96 hour **LC50** = **8.18mg/L** (95% CI 5.85 to 11.4) based upon measured values.

Units/Value:

Results con't

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID). The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

<u>Measured</u>	<u>Fish Total</u>
<u>Conc. (mg/L)</u>	<u>Mortality (@96 hrs)*</u>
Control	0
1.2	0
1.49	0
5.39	2
21.1	10
43.6	10

***10** fish added at test initiation

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences Inc. 1997. Acute Fish Toxicity Test with Rainbow Trout. Study **#164058**.

Other (source):

ExxonMobil Chemicals

Biodegradation

Test Substance: CAS No. 90438-79-2; C6 - C8 branched alkyl acetate ester

Method/Guideline: OECD 301 F

Year (guideline): 1993

Type (test type): Ready Biodegradability, Manometric Respirometry Test

GLP: Yes

Year (study performed): 1998

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep., vessel type, replication, test conditions.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1 L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was **52mg/L**. Sodium benzoate (positive control) concentration was **52mg/L**.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method.**

Test material was readily biodegradable. Half-life was <1 week. By day 28, 77% degradation of the test material was observed. 10% biodegradation was achieved on day 1, 50% biodegradation on approximately day 5.

By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	% Degradation*	Mean % Degradation
	<u>(day 8)</u>	<u>(day 28)</u>
Test Material	73.5, 80.4, 77.4	77.1
Na Benzoate	76.0, 78.3	77.1

* replicate data

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1998 Ready Biodegradability, Manometric Respirometry. Study #1 64094A.

Other (source): ExxonMobil Chemicals

Stability in Water

Test Substance:	CAS No. 90438-79-2; C6 • C8 branched alkyl acetate ester
Method/Guideline:	OECD Guideline 111 and EC Annex V Guideline C.7
Year (guideline):	1992
Type (test type):	Hydrolysis (abiotic)
GLP:	Yes
Year (study performed):	1997
Exposure Period:	17-83 days
Test Conditions:	<p>The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test at pH values of 4, 7, and 9 showed stability at pH 4. A definitive test was performed at pH values of 7 and 9 at varying temperatures (20 and 30 Deg C for pH 9; 40 and 50 Deg C for pH 7). A sufficient volume of test substance stock solution was added to a buffer solution to yield a nominal concentration of less than 60 ug/ml (less than half of expected maximum water solubility concentration). Test samples were stored in the dark in laboratory incubators and the temperature recorded daily.</p> <p>Test vessels were sterilized VOA vials containing a buffer solution with the test substance and no headspace.</p> <p>Test substance concentrations were measured by GC-FID.</p>
Results:	
Units/Value:	<p>Half life at 50 Deg C and pH 7 = 24.3 days Half life at 40 Deg C and pH 7 = 46.5 days Half life at 30 Deg C and pH 9 = 5.29 days Half life at 20 Deg C and pH 9 = 15.8 days</p>
• Note: Deviations from protocol or guideline, analytical method.	<p>Test substance was stable at pH 4. Less than 10% degradation was measured over a period of 5 days.</p> <p>Hydrolysis of test substance occurred at pH 9, with a slower but measurable rate at pH 7.</p>
Conclusion:	Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 20 Deg C and the pH is at or below 7.
Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1995 Hydrolysis as a Function of pH. Study #1 64090H.
Other (source):	ExxonMobil Chemicals

Fish Acute Toxicity

Test Substance: CAS No. 108419-32-5, C7 - C9 branched alkyl acetate ester

Method/Guideline: USEPA 560/6-82-002 Environmental Effects Test Guideline

Year (guideline): 1982

Type (test type): Flow-Through Fish Acute Toxicity Test

GLP: Yes

Year (study performed): 1985

Species: Fathead Minnow (*Pimephales promelas*)

Analytical Monitoring: Yes (TC)

Exposure Period: 96 hour

Statistical Method: Probit procedure by Litchfield & Wilcoxon

Test Conditions:

- **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

A stock water accommodated fraction (WAF) was prepared by adding 267ml of the test substance to ~40L of laboratory blend water in a glass carboy. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 4.4, 8.8, 17.5, 35.0, and 70.0 % WAF, which measured NA, 1.39, 2.71, 4.90, 9.91, 19.86 mg/L as Total Carbon (TC). The test chambers were glass culture dishes (150 x 75mm). Two replicates with ten fish each were tested per treatment level. Test temperature was 20.96 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.

Dilution water hardness was 159 mg/L as CaCO₃.

The pH ranged from 7.3 to 8.1. Dissolved Oxygen ranged from 6.7 to 8.4 mg/L.

Fish were supplied by in-house laboratory; age = 13 weeks; mean wt.=0.257g; mean total length=2.4cm; test loading=0.21 g of fish/L per 24 hour period.

Results:

Units/Value:

Results con't

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

96 hour **LL50** = 49.5 % WAF (95% CI 46.26 to 52.97) based upon nominal values.

96 hour **LC50** = 14.9 mg/L (95% CI 9.91 to 20.0) based upon measured TC values.

Analytical method used was Total Carbon (TC). TC values represent the mean of samples taken on days 0, 2 and 4 less the control value, which was not reported. The **LC50** values based upon TC and were re-calculated in 1994 and issued in an amended report.

<u>Measured</u> <u>Conc. (mg/L of TC)</u>	<u>Fish Total</u> <u>Mortality_(@96_hrs)</u>
Control	0
1.39	0
2.71	0
4.90	0
9.91	0
19.86	20

*20 fish added at test initiation

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test. Study #230341.

Other (source):

ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance: CAS No.108419-32-5; C7 ■ C9 branched alkyl acetate ester

Method/Guideline: USEPA TSCA

Year (guideline) 1992

Type (test type): A Flow-Through Daphnia Acute Toxicity Test

GLP: Yes

Year (study performed): 1985

Species: Water Flea (Daphnia magna)

Analytical Monitoring: Yes (TC)

Exposure Period: 48 hour

Statistical Method: Finney, D.J. **probit** procedure of SAS

Test Conditions:

- **Note: Concentration` prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

A stock water accommodated fraction (WAF) was prepared by combining test substance with laboratory dilution water, at a ratio of 6.7ml per liter of water. The total volume prepared was not reported. The mixture was stirred for 72 hours and the 100% WAF was drawn out via a siphon tube and used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless steel, with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF, which measured: NA, 1.87, 4.13, 10.24, 20.21, and 39.95mg /L as Total Carbon (TC). The test chambers were glass tanks with approximately 6L of test solution flowing through over a 24-hour period. Two replicates with ten daphnids each were tested per treatment level.

Test temperature was 21.36 +/- 0.39 Deg. C. Lighting was 16 hours dark and 8 hour light with gradual on/off periods and an intensity of 83 to 87 ft candles.

Dilution water hardness was 157 mg/L measured as CaCO₃. Dissolved oxygen was 7.9 to 8.8mg/L. The pH ranged from 7.5 to 8.1.

Organisms were supplied by in-house cultures; age = <24 hours old.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

48 hour EC50 = 73.58 % WAF (95% CI 62.18 to 89.3 % WAF) based upon nominal values.

48 hour EC50 based upon measured values was 29.4 mg TC/L. (95% CI 24.6 to 36.3 mg TC/L)

Analytical method used was Total Carbon (TC). Measured TC values are based upon the mean of samples taken on days 0, 1 and 2 less the control value.

<u>Meas. Conc.</u> <u>(mg TC/L)</u>	<u>Daphnia Total</u> <u>Mortality (@48 hrs)</u>
Control	1
1.87	1
4.13	1
10.24	0
20.21	3
39.95	17

*20 Daphids total added at test initiation.

Mortality is defined as immobilized.

EC50 based upon TC is the result of a recalculation in an amended report in 1994.

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

BioDynamics, Inc. 1985. A Flow-Through Acute Daphnia Toxicity Test. Study # 230364.

Other (source):

ExxonMobil Chemicals

Algal Toxicity

Test Substance:	CAS No. 108419-32-5, C7 - C9 branched alkyl acetate ester
Method/Guideline:	USEPA, Environmental Effects Test Guideline EPA 560/6-83-002
Year (guideline):	1983
Type (test type):	Algal Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species/Strain:	Fresh-Water Green Algae (<i>Selenastrum capricornutum</i>)
Analytical Monitoring:	Yes (TC, Total Carbon)
Exposure Period:	96 hour
Statistical Method:	Inverse interpolation method of Snedecor and Cochran
Test Conditions:	<p>A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1 L of algal nutrient media in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separatory funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0×10^4. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at -100 rpm.</p> <p>The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured, NA, 2.78, 5.74, 10.32, 21.46, and 44.71 mg TC/L respectively.</p> <p>Test temperature was 23.99 Deg. C. Lighting was continuous at -4300 Lux (400 ft candles). The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.</p>
• Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.	
Results:	
Units/Value:	72 hour EL50b=20.97mg TC/L (biomass) 72 hour EL50gr=29.65mg TC/L (growth rate)
Measurement (cells/growth)	96 hour EL50b=19.4mg TC/L (biomass) 96 hour EL50gr=43.52mg TC/L (growth rate) NOELRb = 31 .0 mg/L NOELRgr = 8.0 mg/L
	Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples minus the control value (3.375mg TC/L). No excursions from the protocol were noted.

Results con't

Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.

Nominal Conc (%WAF)	Growth Rate 72 & 96 hr. (% Inhibition)		Mean Cell Conc. - 96 hr (cells/ml)
Control	na	na	4.6×10^6
6.25	0.11	1.59	4.0×10^6
12.5	30.24	33.48	2.7×10^6
25.0	2.50	3.33	3.6×10^6
50.0	36.90	34.31	2.5×10^6
100.0	63.51	60.48	1.8×10^5

na - not applicable

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences Inc. 1985. Algal Acute Toxicity Test. Study #230359.

Other (source):

ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance:	CAS No.108419-34-7; C9 - CI 1 branched alkyl acetate ester
Method/Guideline:	OECD 202
Year (guideline)	1984
Type (test type):	A Static Acute Daphnia Toxicity Test
GLP:	Yes
Year (study performed):	1999
Species:	Water Flea (Daphnia magna)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Trimmed Spearman Karber
Test Conditions:	<p>Individual treatment solutions were prepared as water accommodated fractions (WAFs). A WAF was prepared by adding test substance, via syringe, to 2.0L of laboratory dilution water in a glass aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was <10% of solution volume. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle. Test vessels were 125ml glass beakers filled with 140ml of solution and covered (no headspace). Four replicates were prepared for each treatment. Each replicate contained 5 organisms.</p> <p>Nominal treatment levels were; control, 1.3, 3.2, 8.0, 20.0, and 50.0mg/ which measured; ND, 0.44, 1.3, 2.1, 1.9, 2.2mg/L respectively.</p> <p>Test temperature was 20.0 Deg C. Lighting measured 691 Lux with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 6.8 to 8.3mg/L. The pH ranged from 7.2 to 7.6.</p> <p>Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 15 days old.</p>

- Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.

Results:

Units/Value:

48 hour EL50 = **6.7mg/L** (95% CI 5.1 to 8.8) based upon nominal values.

48 hour EC50 based upon measured values was not reported.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was GC-MSD. Measured values are based upon the mean of samples taken on day 0, and day 2.

<u>Nominal. Conc.</u> <u>(mg/L)</u>	<u>Daphnia Total</u> <u>Mortality (@48 hrs)*</u>
Control	0
1.3	0
3.2	4
8.0	11
20.0	19
50.0	20

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences, Inc. 2000. Daphnia Acute Immobilization Test. Study # 129942.

Other (source):

ExxonMobil Chemicals

Biodegradation

Test Substance:	CAS No. 108419-34-7; C9 - Cl 1 branched alkyl acetate ester													
Method/Guideline:	OECD 301 F													
Year (guideline):	1993													
Type (test type):	Ready Biodegradability, Manometric Respirometry Test													
GLP:	Yes													
Year (study performed):	1995													
Inoculum:	Domestic activated sludge													
Exposure Period:	28 days													
Test Conditions:	<p>Test vessels were electronically monitored for oxygen consumption. Test material was tested in triplicate, while controls and blanks were tested in duplicate.</p> <p>Test material concentration was approximately 45mg/L. Sodium benzoate (positive control) concentration was 50mg/L. The inoculum was not acclimated.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p> <p>Data were provided in a summary report, in which details of treatment preparation, media, vessel size, and temperature were not reported. However, the test procedure followed the OECD 301 F test guideline.</p>													
• Note: Concentration prep., vessel type, replication, test conditions.														
Results:														
Units/Value:	<p>Test material was readily biodegradable. Half-life was 1 week. By day 28, 85% degradation of the test material was observed. 10% biodegradation was achieved on day 2, 50% biodegradation on approximately day 7.</p> <p>By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted.</p> <p>Biodegradation was based on oxygen consumption and the theoretical oxygen demand (ThOD) of the test material as calculated using results of an elemental analysis of the test material.</p>													
• Note: Deviations from protocol or guideline, analytical method.														
	<table><tr><th></th><th>% Degradation*</th><th>Mean % Degradation</th></tr><tr><th>Sample</th><th>(day 8)</th><th>(day 28)</th></tr><tr><td>Test Material</td><td>81, 92, 81</td><td>84.7</td></tr><tr><td>Na Benzoate</td><td>92, 91</td><td>91.5</td></tr></table>			% Degradation*	Mean % Degradation	Sample	(day 8)	(day 28)	Test Material	81, 92, 81	84.7	Na Benzoate	92, 91	91.5
	% Degradation*	Mean % Degradation												
Sample	(day 8)	(day 28)												
Test Material	81, 92, 81	84.7												
Na Benzoate	92, 91	91.5												
	• replicate data													

Conclusion:

Reliability: (2) Reliable with restrictions

Reference: Exxon Biomedical Sciences Inc. 1996 Ready Biodegradability, Manometric Respirometry. Study #1 29794A.

Other (source): ExxonMobil Chemicals

Fish Acute Toxicity

Test Substance: CAS No. 108419-35-8, Cl 1 - Cl4 branched alkyl acetate ester

Method/Guideline: USEPA 40 CFR 792

Year (guideline): NR

Type (test type): Flow-Through Fish Acute Toxicity Test

GLP: Yes

Year (study performed): 1985

Species: Fathead Minnow (*Pimephales promelas*)

Analytical Monitoring: Yes (TC)

Exposure Period: 96 hour

Statistical Method: Not Applicable

Test Conditions:

- Note: **Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

A stock water accommodated fraction (WAF) was prepared by adding the test substance to laboratory blend water at a ratio of 1:150. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF. The test chambers were 15L glass tanks containing 14L of solution. Two replicates with ten fish each were tested per treatment level.

Test temperature was 21.78 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.

Dilution water hardness was 158 mg/L as CaCO₃.

The pH ranged from 7.6 to 8.0. Dissolved Oxygen ranged from 7.7 to 8.6 mg/L.

Fish were supplied by in-house laboratory; age = 25 weeks; mean wt.=0.276g; mean total length=2.5cm; test loading=0.023g of fish/L per 24 hour period.

Results:

96 hour LL_0 = 5800 mg/L.

Units/Value:

Value calculated based upon test substance loading.

The amount of TOC measured (less the control value) was too low to measure.

Results con't

- **Note:** Deviations from protocol or guideline, analytical method, biological observations, control survival.

<u>Nominal</u> <u>Conc. (% WAF)</u>	<u>Fish Total</u> <u>Mortality (@96 hrs)</u>
Control	0
6.25	0
12.5	0
25.0	0
50.0	0
100.0	0

*20 fish added at test initiation

Conclusion:

The test material is considered non-toxic at its level of water solubility.

Reliability:

(1) Reliable without restriction

Reference:

BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test Study #252141.

Other (source):

ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance:	CAS No.108419-35-8; Cl 1 - Cl4 branched alkyl acetate ester
Method/Guideline:	USEPA 560/6-82
Year (guideline)	1984
Type (test type):	A Static Acute Daphnia Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species:	Water Flea (Daphnia magna)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Not Applicable
Test Conditions:	<p>A water accomodated fraction (WAF) was prepared as a stock solution and then diluted to prepare the individual treatment levels. The WAF was prepared by adding 16.75ml of the test substance to 2.5L of laboratory dilution water in a glass carboy and mixed with a magnetic stir plate and bar. After mixing for 72 hours, the 100% WAF was drawn out through a sampling tube. Test vessels were 400ml glass beakers filled with 250ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 10 organisms. Nominal treatment levels were; control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF.</p> <p>Test temperature was 20.92 Deg C. Lighting measured 78 to 85 ft. candles with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.3 to 9.5mg/L. The pH ranged from 8.2 to 8.5 units.</p> <p>Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 13 days old.</p>

• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Results:

48 hour EL₅₀ = 5829 mg/L (based upon calculation of test substance loading.

Units/Value:

- **Note:** Deviations from protocol or guideline, analytical method, biological observations, control survival.

Analytical method used was Total Carbon (TC). The measured TC values (less the controls) were within the variability of the analytical method.

<u>Nominal. Conc.</u>	<u>Daphnia Total</u>
<u>WAF)</u>	<u>Mortality (@48 hrs)*</u>
Control	0
6.25	0
12.5	0
25.0	0
50.0	0
100.0	0

*40 Daphids total added at test initiation.

Mortality is defined as immobilized.

Some daphnids observed swimming on the surface in all treatment levels.

Three trials of the study were performed to confirm study results. Trials 2 and 3 exhibited no toxicity (trial 1 **was** not reported). The third trial is documented here.

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

Exxon Biomedical Sciences, Inc. 1985. An Acute Static Daphnia Toxicity Test. Study # 252142A.

Other (source):

ExxonMobil Chemicals

Algal Toxicity

Test Substance:	CAS No. 108419-35-8, C1 - C14 branched alkyl acetate ester
Method/Guideline:	USEPA, EPA 560/6-83-002
Year (guideline):	1983
Type (test type):	Algal Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species/Strain:	Fresh-Water Green Algae (<i>Selenastrum capricornutum</i>)
Analytical Monitoring:	Yes (TC, Total Carbon)
Exposure Period:	96 hour
Statistical Method:	Not Applicable
Test Conditions:	<p>A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1 L of algal nutrient media (AAP) in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separator-y funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0×10^4. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at 100 rpm. The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured (less the control value) na, 0, 0.058, 0.219, 0.492, and 0.873ppm of TC.</p> <p>Test temperature was 23.89 Deg. C. Lighting was continuous at 400 ft candles. The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.</p>
• Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.	
Results:	
Units/Value:	96 hour EL_{50} : = 5829 mg/L 96 hour EL_{01} : = 5829 mg/L
Measurement (cells/growth)	$NOELR_b$ = 5829 mg/L $NOELR_{gr}$ = 5829 mg/L No Inhibition of Algal growth was observed at the highest treatment level 100% WAF (0.873 ppm Carbon). Concentration re-calculated based upon loading of test substance. Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples less the control value on day 0 of the study. No excursions from the protocol were noted.

Results con't

Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.

Nominal
Conc. (%WAF)
 Control
 6.25
 12.5
 25.0
 50.0
 100.0

Mean Cell
 Conc. • 96 hr
(cells/ml)
 5.2x10⁶
 4.4 x1 0⁶
 4.6 x1 0⁶
 4.1 x10⁶
 5.3 x1 0⁶
 5.2 x1 0⁶

Conclusion:

Reliability:

(1) Reliable without restriction

Reference:

BioDynamics, Inc. 1985. An Acute Algal Toxicity Test. Study #252159.

Other (source):

ExxonMobil Chemicals

Biodegradation

Test Substance: CAS No. 108419-35-8; Cl 1 - Cl4 branched alkyl acetate ester

Method/Guideline: USEPA EPA 560/6-83-003, CG-2000

Year (guideline): 1982

Type (test type): Aerobic Aquatic Biodegradation

GLP: Yes

Year (study performed): 1985

Inoculum: Acclimated media

Exposure Period: 28 days

Test Conditions:

- **Note: Concentration prep., vessel type, replication, test conditions.**

The inoculum was acclimated to the test substance for 14 days prior to study initiation. The media consisted of mineral salt solutions, pond sediment, activated sludge, distilled water, and small amounts (10ul) of test substance. The media was mixed and placed on a gyratory shaker in the dark for 13 days. After settling overnight the supernatant was pour off and was used as the inoculum for the test phase.

The test system utilized 2.0L Glenhill flasks as test vessels. Approximately 13.0mg of test substance were added to 900ml of glass distilled water. Additionally, 1 00ml of acclimated media and 1 ml of mineral salts were added. The flasks were sealed and placed on a gyratory shaker in the dark. Three replicates of the test substance were evaluated. Twice a week, the flasks were monitored for spent NaOH and titrated for carbon dioxide (CO₂). Total Organic Carbon (TOC) was measured at initiation and termination in the controls.

A positive and negative control were tested consisting of Phthalic acid (100ml at 103.8mg/L) and HgC12 (10 ml at 51g/L) respectively, along with three blanks.

Test temperature ranged from 21.5 to 25.0 Deg C.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

The test material was not readily biodegradable. By day 28, 31% degradation of the test material was observed. The half-life, and 10% biodegradation achievement periods were not reported. The positive control (phthalic acid) degraded by 43.8% by day 28, with a TOC removal of 100.7%. Biodegradation was based on NaOH usage and calculated CO₂ evolution. No excursions from the protocol were noted.

Conclusion:

Reliability:

(2) Reliable with restrictions

TOC values not measured on test treatments only controls. No replicate values reported (mean only).

Reference:

BioDynamics, Inc. 1985 Ultimate Biodegradability, Study # 252189

Other (source):

ExxonMobil Chemicals